Yong Chu 10-02-2007 10/569,159 \$%^STN; HighlightOn=; HighlightOff=; Connecting via Winsock to STN Welcome to STN International! Enter x:x LOGINID: ssptaylc1626 PASSWORD: TERMINAL (ENTER 1, 2, 3, OR ?):2 Welcome to STN International Web Page for STN Seminar Schedule - N. America NEWS 1 JUL 02 LMEDLINE coverage updated NEWS JUL 02 SCISEARCH enhanced with complete author names NEWS 3 JUL 02 CHEMCATS accession numbers revised NEWS 4 CA/CAplus enhanced with utility model patents from China JUL 02 NEWS 5 CAplus enhanced with French and German abstracts NEWS JUL 16 NEWS 7 JUL 18 CA/CAplus patent coverage enhanced USPATFULL/USPAT2 enhanced with IPC reclassification NEWS 8 JUL 26 USGENE now available on STN NEWS 9 JUL 30 CAS REGISTRY enhanced with new experimental property tags NEWS 10 AUG 06 NEWS 11 AUG 06 BEILSTEIN updated with new compounds NEWS 12 AUG 06 FSTA enhanced with new thesaurus edition NEWS 13 AUG 13 CA/CAplus enhanced with additional kind codes for granted patents CA/CAplus enhanced with CAS indexing in pre-1907 records NEWS 14 AUG 20 Full-text patent databases enhanced with predefined NEWS 15 AUG 27 patent family display formats from INPADOCDB AUG 27 USPATOLD now available on STN NEWS 16 CAS REGISTRY enhanced with additional experimental NEWS 17 AUG 28 spectral property data NEWS 18 SEP 07 STN AnaVist, Version 2.0, now available with Derwent World Patents Index NEWS 19 SEP 13 FORIS renamed to SOFIS SEP 13 INPADOCDB enhanced with monthly SDI frequency NEWS 20 CA/CAplus enhanced with printed CA page images from NEWS 21 SEP 17 1967-1998 CAplus coverage extended to include traditional medicine NEWS 22 SEP 17 EMBASE, EMBAL, and LEMBASE reloaded with enhancements NEWS 23 SEP 24 OCT 02 CA/CAplus enhanced with pre-1907 records from Chemisches NEWS 24 Zentralblatt 19 SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2, NEWS EXPRESS CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007. STN Operating Hours Plus Help Desk Availability NEWS HOURS

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chain nodes :

1 2 3

ring nodes :

4 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23

chain bonds :

1-2 1-7 2-3 3-4

ring bonds :

4-12 4-15 7-8 7-11 8-9 9-10 9-16 10-11 10-19 12-13 13-14 13-20 14-15

14-23 16-17 17-18 18-19 20-21 21-22 22-23

exact/norm bonds :

1-2 1-7 2-3 3-4 4-12 4-15 7-8 7-11 8-9 9-10 9-16 10-11 10-19 12-13

13-14 13-20 14-15 14-23 16-17 17-18 18-19 20-21 21-22 22-23

G1:C,O,S,N,Se

Match level :

1:CLASS 2:CLASS 3:CLASS 4:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom

12:Atom

13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom

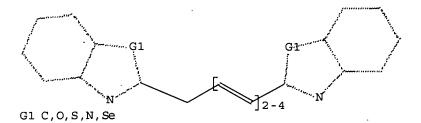
22:Atom 23:Atom

## L1 STRUCTURE UPLOADED

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L1 STR



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SAMPLE SCREEN SEARCH COMPLETED - 990 TO ITERATE

100.0% PROCESSED 990 ITERATIONS

2 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 17913 TO 21687

PROJECTED ANSWERS: 2 TO

L2 2 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 13:37:50 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 20818 TO ITERATE

100.0% PROCESSED 20818 ITERATIONS 27 ANSWERS

124

SEARCH TIME: 00.00.01

L3 27 SEA SSS FUL L1

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=> s 13

L4 10 L3

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L4 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1990:477580 CAPLUS Full-text

DOCUMENT NUMBER:

113:77580

TITLE:

Spectrophotometric studies of acid-base properties of

cationic cyanine dyes

AUTHOR (S):

Balog, I. S.; Kish, P. P.; Ishchenko, A. A.; Mushkalo,

V. L.; Andrukh, V. A.

CORPORATE SOURCE:

SOURCE:

Uzhgorod State Univ., Uzhgorod, USSR

Zhurnal Analiticheskoi Khimii (1990), 45(3), 481-90

CODEN: ZAKHA8; ISSN: 0044-4502

DOCUMENT TYPE:

LANGUAGE:

Journal Russian

GI

Me Me Me Me 
$$(CH = CH)_{\Pi}CH$$
  $NMe_2$  Br-

II

The electronic absorption spectra and protonation and hydrolysis consts. of 12 cationic cyanine dyes, e.g., I (R = Me, CH2CH2OH, CH2CH2OAc; n = 1, 2, 3; X = Cl, Br) and II, were obtained. The dyes exist as reactive, singly charged forms over a wide acidity range. Charge distributions were calcd., and the protolysis mechanism was discussed.

IT 128646-92-4 128646-93-5 128646-95-7

RL: PRP (Properties)

(UV spectrum of)

RN 128646-92-4 CAPLUS

CN 3H-Indolium, 2,2'-(1,3-pentadiene-1,5-diyl)bis[1,3,3-trimethyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N+} \\ \text{CH}_2\text{-CH} \\ \text{CH-CH} \\ \text{CH-CH} \\ \text{CH} \\ \text{Me} \\ \end{array}$$

RN 128646-93-5 CAPLUS

CN 3H-Indolium, 2,2'-(1,3,5-heptatriene-1,7-diyl)bis[1,3,3-trimethyl- (9CI) (CA INDEX NAME)

RN 128646-95-7 CAPLUS

CN 3H-Indolium, 2,2'-(1,3-pentadiene-1,5-diyl)bis[1-(2-hydroxyethyl)-3,3-dimethyl- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1990:181375 CAPLUS Full-text

DOCUMENT NUMBER:

112:181375

TITLE:

N,N-cyanines of a benzo[c,d]indole series and their

anionic dyes

AUTHOR(S):

Vasilenko, N. P.; Maidannik, A. G.; Mikhailenko, F. A.

CORPORATE SOURCE: Inst. org. Khim., Kiev, USSR

SOURCE:

Ukra/nskii Khimicheskii Zhurnal (Russian Edition)

 $(1\cancel{8}89)$ , 55(7), 742-6

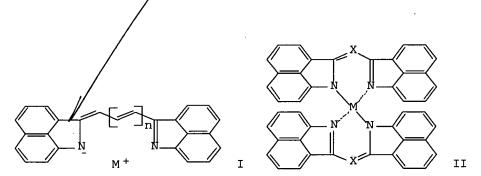
CODEN: UKZHAU; ISSN: 0041-6045

DOCUMENT TYPE:

LANGUAGE:

Journal Russian

GI



The cyanine dyes I (M = Li, Na, K; n = 0,1,2) and II (X = CH, N; M = Zn, Cu, Co, Ni) were prepd. and their spectra were studied with respect to structure. The absorption max. for I (n = 1) was little dependent on the nature of the counterion in THF or in DMSO, indicating the formation of ion pairs in the weakly polar THF. The form of the absorption curves for I anionic dyes, II complex dyes, and their cationic dye analogs was similar, indicating that the benz[c,d]indole chromophore system was responsible for the absorption in all cases.

IT 126667-25-2P 126667-26-3P 126667-27-4P

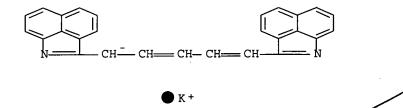
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and spectral properties of)

RN 126667-25-2 CAPLUS

CN Benz[cd]indole, 2,2'-(1,3-pentadiene-1,5-diyl)bis-, ion(1-), lithium (9CI) (CA INDEX NAME)

● Li +

RN 126667-27-4 CAPLUS
CN Benz[cd]indole, 2,2'-(1,3-pentadiene-1,5-diyl)bis-, ion(1-), potassium
(9CI) (CA INDEX NAME)



L4 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 1990:38114 CAPLUS Full-text

DOCUMENT NUMBER: 11/2:38114

TITLE: Dimerization reactions of cyanine radical dications

AUTHOR(S): Parton, R. L.; Lenhard, J. R.

CORPORATE SOURCE: / Res. Lab., Eastman Kodak Co., Rochester, NY, 14650,

USA

SOURCE: Journal of Organic Chemistry (1990), 55(1), 49-57

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal LANGUAGE: English

AB Radical dications formed during the one-electron oxidn. of representative cationic dicarbocyanine (pentamethine) dyes lacking alkyl substitution on the even-numbered carbon atoms of the methine chain underwent irreversible

dimerization in MeOH or MeCN soln. Deprotonation of the resultant UV-absorbing dimer gave a dicationic bis-dye with spectral properties similar to those of the parent dye. These bis-dyes were susceptible to further oxidn. via a reversible two-electron mechanism to yield a highly unsatd., cross-conjugated, tetracationic species. The chem. of radical dications derived from the one-electron oxidn. of carbocyanine (trimethine) dyes depended on the nature of the dye heterocycle as well as the degree of alkyl substitution in the methine chain. Some thiacarbocyanine radical dications irreversibly dimerized and gave products analogous to those obsd. for dicarbocyanines. A persistent radical dication was obtained by the one-electron oxidn. of an indolocarbocyanine and a chain-substituted thiacarbocyanine dye.

IT 123811-94-9P 123812-04-4P 123812-06-6P

123834-26-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and spectral properties of)

RN 123811-94-9 CAPLUS

Benzothiazolium, 2,2',2''-[3-[2-(3-ethylbenzothiazolium-2-yl)ethenyl]-1,3,5,7-octatetraene-1,4,8-triyl]tris[3-ethyl-, tetrakis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

CM 1

CN

CRN 123811-93-8 CMF C46 H44 N4 S4

CM 2

CRN 16919-18-9 CMF F6 P

CCI CCS

RN 123812-04-4 CAPLUS

CN Benzoxazolium, 2,2',2''-[3-[2-(3-ethylbenzoxazolium-2-yl)ethenyl]-1,3,5,7-octatetraene-1,4,8-triyl]tris[3-ethyl- (9CI) (CA INDEX NAME)

RN 123812-06-6 CAPLUS

CN Benzoselenazolium, 2,2',2''-[3-[2-/3-ethylbenzoselenazolium-2-yl)ethenyl]-1,3,5,7-octatetraene-1,4,8-triyl]tris[3-ethyl- (9CI) (CA INDEX NAME)

RN 123834-26-4 CAPLUS

CN 3H-Indolium, 2,2',2''-[3-[2-(1-ethyl-3,3-dimethyl-3H-indolium-2-yl)ethenyl]-1,3,5,7-octatetraene-1,4,8-triyl]tris[1-ethyl-3,3-dimethyl-,tetrakis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

CM 1

CRN 123834-25-3 CMF C58 H68 N4

CM

CRN 16919-18-9

CMF F6 P CCI CCS

CAPLUS COPYRIGHT 2007 ACS on STN ANSWER 4 OF 10

ACCESSION NUMBER: 1977:185307 CAPLUS Full-text

DOCUMENT NUMBER:

86:18/5307

TITLE: AUTHOR(S): Thip-layer chromatography of some cyanine dyes

CORPORATE SOURCE:

Kues, H. A.; Teague, C. E.

SOURCE:

Appl. Phys. Lab., Johns Hopkins Univ., Laurel, MD, USA

 $\Delta$  ournal of Chromatography (1977), 135(1), 221-5

CODEN: JOCRAM; ISSN: 0021-9673

DOCUMENT TYPE:

LANGUAGE:

Journal English

Various thin-layer chromatog. methods, as described by E. Stahl (1969), were tested on different subgroups of cyanine dyes, and RF values and dye purities were detd. Thromatog. was performed on silica gel sheets (100-.mu.m coating) and Al-backed smilica gel sheets (250 .mu.m) with detection by white or UV The best results were obtained with the solvent systems 100% MeOH and PrOH-HCO2H (80:20). The 2 silica gel coatings, although showing some differences in a few cases, produced good reproducibilities.

IT 60683-97-8

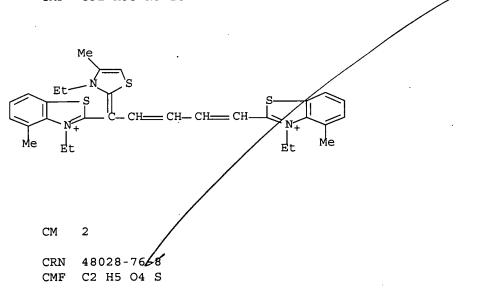
RL: ANT (Analyte); ANST (Analytical study)

(chromatog. of, thin-layer, purity in relation to)

RN 60683-97-8 CAPLUS

Benzothiazolium, 2,2'-[5-(3-ethyl-4-methyl-2(3H)-thiazolylidene)-1,3-CN pentadiene-1,5-diyl]bis[3-ethyl-4-methyl-, bis(ethyl sulfate) (9CI) (CA INDEX NAME)

CRN 60683-96-7 CMF C31 H35 N3 S3



Et - 0- SO3 -

L4 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1977:107984 CAPLUS Full-text

DOCUMENT NUMBER:

86:107984

TITLE:

Direction of polymethine dye protonation

AUTHOR(S):

Tolmachev, A. I.; Kornilov, M. Yu.; Karaban, E. F.

CORPORATE SOURCE:

Inst. Org. Khim., Kiev, USSR

SOURCE:

Teoreticheskaya i Eksperimental'naya Khimiya (1976),

12(6), 817-21

CODEN: TEKHA4; ISSN: 0497-2627

DOCUMENT TYPE:

Journal

LANGUAGE:

Russian

GI

AB The UV and visible spectra and 1H NMR spectra of CF3CO2H solns. of cyanine homologs I (n = 0-3, X = Cl, iodine) and II (n = 0-3; X = O, S) and of model compds. showed that protonation occurred at the CH adjacent to the heterocyclic ring.

IT 62077-45-6

RL: PRP (Properties)

(NMR and UV and visible spectra of)

RN 62077-45-6 CAPLUS

CN Benzothiazolium, 2,2'-(1,3,5-heptatriene-1,7-diyl)bis[3-methyl- (9CI) (CA INDEX NAME)

IT 62077-44-5

RL: PRP (Properties)

(NMR and UV spectra of)

RN 62077-44-5 CAPLUS

CN Benzothiazolium, 2,2'-(1,3-pentadiene-1,5-diyl)bis[3-methyl- (9CI) (CA INDEX NAME)

L4 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1976:572360 CAPLUS Full-text

DOCUMENT NUMBER:

85:172360

TITLE:

Dyes can be deadly

AUTHOR (S):

Kues, Henry A.; Lutty, Gerard A.

CORPORATE SOURCE:

Appl. Phys. Lab., Johns Hopkins Univ., Baltimore, MD,

USA

SOURCE:

Laser Focus (Newton, Massachusetts) (1975), 11(5),

59-61

CODEN: LAFOAK; ISSN: 0023-8589

DOCUMENT TYPE:

Journal

LANGUAGE:

English

GI

AB Of various dyes tested, cyanine and carbocyanine compds. were the most toxic as evidenced by the LD100 value and survival time in mice after injection into the abdominal cavities. The 24-hr LD100 value of 3,3'-dioctadecyl-2,2'-oxacarbocyanine p-toluenesulfonate (I) [60711-74-2] was 5 mg/kg.

IT 60683-97-8

RL: ADV (Adverse effect, including toxicity); BIOL (Biological study) (toxicity of)

RN 60683-97-8 CAPLUS

CN Benzothiazolium, 2,2'-[5-(3-ethyl-4-methyl-2(3H)-thiazolylidene)-1,3-pentadiene-1,5-diyl]bis[3-ethyl-4-methyl-, bis(ethyl sulfate) (9CI) (CA INDEX NAME)

CM 1

CRN 60683-96-7 CMF C31 H35 N3 S3

'Et - 0- SO3 -

L4 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1951:18578 CAPLUS

DOCUMENT NUMBER: 45:18578

ORIGINAL REFERENCE NO.: 45:3273f-i,3274a-b

TITLE: Improvements in carbocyanine photographic sensitizing

dyes

INVENTOR(S): Kendall, John D.; Doyle, Frank P.

PATENT ASSIGNEE(S): Ilford Ltd.

DOCUMENT TYPE: Patent

Unavailable LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

DATE PATENT NO. KIND DATE APPLICATION NO. \_\_\_\_\_\_ -----US 1948-30976 19480603 19501219 US 2534913

For diagram(s), see printed CA Issue. GI

Dye intermediates of the general type, D1.N(R)(A):(CH.CH)n:CCH:CHC(:CHSR'')AΒ )C:(CH.CH)n:N(R')(X)D2, prepd. as described in Brit. 638,023 (cf. following abstr.), in which n is zero, D1 and D2 are the same or different and represent residues of 5-membered heterocyclic systems, R and R' are the same or different and are alkyl, hydroxyalkyl, aralkyl, or hydroxyaralkyl groups, R'' is an alkyl or aralkyl group, and A and X are acid radicals, are treated with solvolytic agents, e.g. H2O or an alc., to give photographic sensitizing dyes, D1.N(R).C:CHCH:C(CHO).C:N(R')(X)D2, or the isomer in which the -CHO is attached at the C atom nearer to the D1 ring. Isolation of the intermediates is not necessary. Reaction mixts. from the process, described in Brit. 638,023, contg. the required intermediate may be treated directly with the solvolytic reagent, reaction occurring either upon allowing the reagents to stand together or upon warming (as long as 30 min. may be required). 3,3'-Diethylthiacarbocyanine iodide 4.9 p-MeC6H4SO3H 2.5, HC(SEt)3 2.5, and Ac2O 25 parts by wt. are refluxed until bright, yellow-orange (approx. 5 min.). Removing the solvent under reduced pressure, washing the residue with Et2O, dissolving in EtOH, and pouring into aq. KI soln. gives 3,3'-diethyl-8formylthiacarbocyanine iodide, crystn. from MeOH, orange with a green reflex, m. 253.degree. (decompn.), also prepd. by use of 2.0 parts HC(SMe)3 or 4.0 parts (PhCH2S)3CH in place of HC(SEt)3; in a gelatinous Ag iodobromide emulsion it imparts a sensitivity band extending to 5800 A., with a sharp max. at 5500 A. The following dyes are prepd. similarly: 3,3'-diethyl-8-formyl-4,5,4',5'-benzobenzoxacarbocyanine iodide, red crystals from MeOH, m. 278.degree. (decompn.); 3,3'-diethyl-8-formylselenocarbocyanine iodide, brown glistening crystals from MeOH, m. 256.degree. (decompn.), sensitivity band to 6000 A., max. about 5400 A.; 3,3'-diethyl-5,5'-dimethyl-8formylthiacarbocyanine iodide, red-brown, crystals from MeOH, m. 265.degree. (decompn.), sensitivity band to 6000 A., max. about 5500 A.; 3,3'-diethyl-5,5'-dichloro-8-formyl- thiacarbocyanine iodide, brown powder, m. 298.degree. (decompn.); 3,3'-diethyl-4,5,4',5'-dibenzo-8-formylthiacarbocyanine iodide, brown needles from MeOH, m. 302.degree. (decompn.). 878787-03-2P, Benzothiazolium, 2,2'-[5-[2-(1,3,3-trimethyl-2indolinylidene) ethylidene] -1,3-pentadienylene] bis[3-ethyl-5-methyliodide] 878787-04-3P, Benzothiazolium, 2,2'-[5-[2-(1,3,3-

trimethyl-2-indolinylidene)ethylidene]-1,3-pentadienylene]bis[5-chloro-3ethyl-, iodide RL: PREP (Preparation)

(prepn. of)

RN 878787-03-2 CAPLUS

Benzothiazolium, 2,2'-[5-[2-(1,3,3-trimethyl-2-indolinylidene)ethylidene]-CN 1,3-pentadienylene]bis[3-ethyl-5-methyl-iodide] (5CI) (CA INDEX NAME)

RN878787-04-3 CAPLUS

CNBenzothiazolium, 2,2'-[5-[2-(1/,3,3-trimethyl-2-indolinylidene)ethylidene]-1,3-pentadienylene]bis[5-chlqro-3-ethyl-, iodide (5CI) (CA INDEX NAME)

ANSWER 8/OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1951:18577 CAPLUS

DOCUMENT NUMBER:

45:18577

ORIGINAL REFERENCE NO.:

45:3273f-i,3274a-b

TITLE:

Improvements in carbocyanine photographic sensitizing

INVENTOR(S):

Kendall, John D.; Doyle, Frank P.

PATENT ASSIGNEE(S):

Ilford Ltd.

DOCUMENT TYPE:

Patent

LANGUAGE:

FAMILY ACC. NUM. COUNT:

Unavailable

PATENT INFORMATION:

PATENT NO. KIND APPLICATION NO. DATE GB 638022 19500531 GB 1947-14792 19470604

GI For diagram(s), see printed CA Issue.

AB Dye intermediates of the general type, D1.N(R)(A):(CH.CH)n:CCH:CHC(:CHSR'' )C:(CH.CH)n:N(R')(X)D2, prepd. as described in Brit. 638,023 (cf. following abstr.), in which n is zero, D1 and D2 are the same or different and represent residues of 5-membered heterocyclic systems, R and R' are the same or different and are alkyl, hydroxyalkyl, aralkyl, or hydroxyaralkyl groups, R'' is an alkyl or aralkyl group, and A and X are acid radicals, are treated with solvolytic agents, e.g. H2O or an alc., to give photographic sensitizing dyes, D1.N(R).C:CHCH:C(CHO).C:N(R')(X)D2, or the isomer in which the -CHO is

attached at the C atom nearer to the D1 ring. Isolation of the intermediates is not necessary. Reaction mixts. from the process, described in Brit. 638,023, contg. the required intermediate may be treated directly with the solvolytic reagent, reaction occurring either upon allowing the reagents to stand together or upon warming (as long as 30 min. may be required). Diethylthiacarbocyanine iodide 4.9 p-MeC6H4SO3H 2.5, HC(SEt)3 2.5, and Ac2O 25 parts by wt. are refluxed until bright, yellow-orange (approx. 5 min.). Removing the solvent under reduced pressure, washing the residue with Et2O, dissolving in EtOH, and pouring into aq. KI soln. gives 3,3'-diethyl-8formylthiacarbocyanine iodide, crystn. from MeOH, orange with a green reflex, m. 253.degree. (decompn.), also prepd. by use of 2.0 parts HC(SMe)3 or 4.0 parts (PhCH2S)3CH in place of HC(SEt)3; in a gelatinous Ag iodobromide emulsion it imparts a sensitivity band extending to 5800 A., with a sharp max. at 5500 A. The following dyes are prepd. similarly: 3,3'-diethyl-8-formyl-4,5,4',5'-benzobenzoxacarbocyanine iodide, red crystals from MeOH, m. 278.degree. (decompn.); 3,3'-diethyl-8-formylselénocarbocyanine iodide, brown glistening crystals from MeOH, m. 256.degree. (decompn.), sensitivity band to 6000 A., max. about 5400 A.; 3,3'-diethyl-5,5'-dimethyl-8formylthiacarbocyanine iodide, red-brown, grystals from MeOH, m. 265.degree. (decompn.), sensitivity band to 6000 A., max. about 5500 A.; 3,3'-diethyl-5,5'-dichloro-8-formyl- thiacarbocyaning iodide, brown powder, m. 298.degree. (decompn.); 3,3'-diethyl-4,5,4',5'-dibénzo-8-formylthiacarbocyanine iodide, brown needles from MeOH, m. 302.degree. (decompn.).

IT 878787-03-2P, Benzothiazolium, 2,2'-[5-[2-(1,3,3-trimethyl-2-indolinylidene)ethylidene]-1,3-pentadienylene]bis[3-ethyl-5-methyl-iodide] 878787-04-3P, Benzothiazolium, 2,2'-[5-[2-(1,3,3-trimethyl-2-indolinylidene)ethylidene]-1,3-pentadienylene]bis[5-chloro-3-ethyl-, iodide

RL: PREP (Preparation) (prepn. of)

RN 878787-03-2 CAPLUS

CN Benzothiazolium, 2,2'-[5-[2/(1,3,3-trimethyl-2-indolinylidene)ethylidene]-1,3-pentadienylene]bis[3-ethyl-5-methyl-iodide] (5CI) (CA INDEX NAME)

RN 878787-04-3 CAPLUS

CN Benzothiazolium, 2,2'-[5-[2-(1,3,3-trimethyl-2-indolinylidene)ethylidene]-1,3-pentadienylene]bis[5-chloro-3-ethyl-, iodide (5CI) (CA INDEX NAME)

L4 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1951:15913 CAPLUS

DOCUMENT NUMBER: 45:15913

ORIGINAL REFERENCE NO.: 45:2803d-i,2804a

TITLE: Cyanine dye intermediates

INVENTOR(S): Kendall, John D.; Doyle, Frank P.

PATENT ASSIGNEE(S): Ilford Ltd.

DOCUMENT TYPE: Patent LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

AB

GI For diagram(s), see printed CA Issue.

Cyanine dye intermediates, used in the synthesis of trinuclear polymethine photographic emulsion sensitizers, are prepd. from cyanine dyes and are believed to have the structure D'.N/R')(A):(CH.CH)n:C(CH:CH)xC(:CHSR''')C: (CH.CH)n:N(R'')(X).D'', where R' and R'' are alkyl, hydroxyalkyl, aralkyl, or hydroxyaralkyl groups, D' and D''/are residues of 5- or 6-membered heterocyclic nuclei, n is 0 or 1/, x is 1 or 2, A and X are acid radicals, and R''' is an alkyl or aralkyl gro⁄up. Thus, 1,1'-diethyl-2,2'- quinocarbocyanine iodide 4.8, p-toluenesulfonic acid 2.5, and triethyltrithio orthoformate 2.2 parts refluxed in acetic anhydride, the excess solvent removed by evapn. in vacuo, washed with Et2O, digsolved in EtOH, poured into aq. KI soln., the filtered ppt. washed with H2O followed by EtOH, and crystd. from EtOH yields orange-red needles of 1-(éthylmercapto)-2,4-di-2-quinolyl-1,3-butadiene di-EtI, m. 176.degree. (decompn.). The following dye intermediates were prepd. in a similar manner: 1-/(ethylmercapto)-2,4-bis(2-benzothiazolyl)-1,3-butadiene bis(Et p-toluenesulfonáte), 1-(ethylmercapto)-2,4-bis(2-benzothiazolyl)-1,3butadiene EtI Et p-toluenesulfonate (a hygroscopic yellow solid), 1-(methylmercapto)-2,4-bis(2-benzothiazolyl)-1,3-butadiene bis(Et ptoluenesulfonate), 1-(benzylmercapto)-2,4-bis(2-benzothiazoly1)-1,3- butadiene bis(Et p-toluenesulfonate), 1-(ethylmercapto)-2,4-bis(5-methyl-2benzothiazolyl)-1,3-butadiene Et p-toluenesulfonate EtI 1-(ethylmercapto)-2,4bis(5-methyl-2-benzothiazolyl)-1,3-butadiene di-EtI, m. 254.degree. (decompn.), 1-(ethylmercapto)-2,4-bis(5-chloro-2- benzothiazolyl)-1,3butadiene bis(Et p-toluenesulfonate). 1-(ethylmercapto)-2,4-bis(5-chloro-2benzothiazolyl)-1,3-butadiene di-EtI, m. 190.degree. (decompn.), 1-(ethylmercapto) -2,4-bis(4',5'- benzbenzothiazol-2-yl)-1,3-butadiene bis(Et ptoluenesulfonate), 1-(ethylmercapto)-2,4-bis(4',5'-benzbenzothiazol-2-yl)-1,3butadiene di-EtI, 1-(benzylmercapto)-2,4-bis(4',5'-benzbenzothiazol-2-yl)-1,3butadiene bis(Et p-toluenesulfonate), m. 80.degree. (decompn.), 1(ethylmercapto)-2,4-di-2-quinolyl-1,3-butadiene di-EtBr, 1-(ethylmercapto)-2,4-di-2-quinolyl-1,3-butadiene EtBr Et 2-naphthalenesulfonate, 1-(ethylmercapto)-2,4-di-4-quinolyl-1,3-butadiene EtBr Et p-toluenesulfonate, 1-(ethylmercapto)-2,4-di-4-quinolyl-1,3-butadiene di-EtI m. 283.degree. (decompn.), 1-(ethylmercapto)-2,4-di-2- benzoselenazolyl-1,3-butadiene bis(Et p-toluenesulfonate), 1-(ethylmercapto)-2,6-bis(3,3-dimethyl-3H-pseudoindolyl)-1,3,5-hexatriene MeI Me p-toluenesulfonate, 1-(ethylmercapto)-2,6-bis(5-methyl-2- benzothiazolyl)-1,3,5-hexatriene EtI Et p-toluenesulfonate, 1-(ethylmercapto)-2,6-bis(5-chloro-2-benzothiazolyl)-1,3,5-hexatriene EtI Et p-toluenesulfonate, and 1-(ethylmercapto)-2,4-di-2-benzothiazolyl-1,3- butadiene bis(Et p-toluenesulfonate).

IT 857395-00-7P, Pseudoindolium, 2,2'-[5-[(ethylthio)methylene]-1,3-pentadienylene]bis[1,3,3-trimethyl-3H-], iodide, p-toluenesulfonate RL: PREP (Preparation)

(prepn. of)

RN 857395-00-7 CAPLUS

CN Pseudoindolium, 2,2'-[5-[(ethylthio)methylene]-1,3pentadienylene]bis[1,3,3-trimethyl-3H-], iodide, p-toluenesulfonate (5CI)
(CA INDEX NAME)

CM 1

CRN 857394-99-1 CMF C30 H36 N2 S

CM 2

CRN 16722-51-3 CMF C7 H7 O3 S

L4 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1951:7536 CAPLUS

DOCUMENT NUMBER: 45:7536

ORIGINAL REFERENCE NO.: 45:1350e-i,1351a-f

TITLE: Cyanine dyes

INVENTOR(S): Kendall, John D.; Doyle, Frank P.

PATENT ASSIGNEE(S): Ilford Ltd.

DOCUMENT TYPE: Patent LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

KIND

DATE

APPLICATION NO.

DATE

PATENT NO.

------US 2518476 19500815 AB 1-Ethylmercapto-2,4-dibenzothiazolyl-1,3-butadiene dietho-p- toluenesulfonate 2.7 and 2-methylbenzothiazole-EtI (I) 1.5 were heated in anhyd. C5H5N 20 parts for 10 min., the blue soln. was added to aq. KI, dild. with H2O, and cooled to give green bis-2-(3-ethylbenzothiazole) - .gamma.,2'-(3ethylbenzothiazole)pentamethinecyanine diiodide, m. 247.degree. (from MeOH) (all m.ps. are with decompn.). Other products were similarly prepd. with corresponding intermediates and reagents such as I (read dye, color, m.p. and reagent). 2-(3-Ethylbenzothiazole)-2'-(1- ethylquinoline)-.gamma.,2''-(3ethylbenzothiazole) pentamethinecyanine diiodide, green needles, 236.degree., quinaldine-EtI (II); 2'-(3-ethylbenzoxazole) analog, green, 190.degree., 2methylbenzoxazole- EtI (III); 2'-(1,3,3-trimethylindolenine) analog, brassy green, 184.degree., 1,3,3-trimethyl-2-methyleneindolenine; bis-2-(3-ethyl-5methylbenzothiazole) - .gamma.,2'-(3-ethyl-5-methylbenzothiazole)pentamethin ecyanine diiodide, green, m. 248.degree., 2,5-dimethylbenzothiazole-EtI; 2-(3ethyl-5-methylbenzothiazole)-2-(1,3,3-trimethylindolenine) analog, green, 192.degree., 1,3,3-trimethyl-2-methylenedihydroindolenine; bis-2-(3-ethyl-5chlorobenzothiazole) - .gamma., 2' - (3-ethyl-5chlorobenzothiazole) pentamethinecyanine diiodide, golden, 260.degree., 2methyl-5-chlorobenzothiazole-EtI; bis-2-(1-ethylquinoline)-.gamma.,2''- (1ethylquinoline)pentamethinecyanine diiodide, yellow-green, 236.degree., II; and bis-2-(3-ethylbenzoselenazole)-.gamma.,2'-(3ethylbenzoselenazole) pentamethinecyanine monoiodide mono-p- toluenesulfonate, bright green, 245.degree., 2-methylbenzoselenazole-EtI. Tetramethine merocyanines were prepd. similarly: [2-(3-ethylbenzothiazole)- 5'-(3-ethyl-2thio-4-ketotetrahydrothiazole) - .gamma., 2''-(3ethylbenzothiazole)tetramethinemerocyanine] iodide, green, 246.degree., 3ethyl-2-thio-4-ketothiazolidene (IV); 5'-(3-methyl) analog, coppery green, 242.degree., 3-Me analog (V) of IV; 4'-(1-phenyl-3-methyl-5- pyrazolone) analog, green, 194.degree., 1-phenyl-3-methyl-5-pyrazolone (VI); [2-(3-ethyl-5-methylbenzothiazole)-5'-(3-methyl-2-thio-4-keto- tetrahydrothiazole)-.gamma.,2''-(3-ethyl-5-methylbenzothiazole)tetramethin emerocyanine] iodide, golden, 212.degree., V; 5'-(3-ethyl) analog, blue-green, 210.degree., IV; 4'-(1-phenyl-3-methyl-5-pyrazolone) analog, brown-green, 258.degree., VI; [2-(3ethyl-5-chlorobenzothiazole)-5'-(3- methyl-2-thio-4-ketotetrahydrothiazole)-.gamma.,2''-(3-ethyl-5- chlorobenzothiazole)tetramethinemerocyanine] iodide, dark green, 210.degree., V; 5'-(3-ethyl) p-toluenesulfonate analog, yellowgreen, 236.degree., IV; 4'-(1-phenyl-3-methyl-5-pyrazolone) analog, brassy green, 258.degree. (from C5H5N-MeOH), VI; [2-(3-ethyl-4,5benzobenzothiazole) -5'- (3-ethyl-2-thio-4-keto-tetrahydrothiazole) -.gamma.,2''-(3-ethyl-4,5- benzobenzothiazole)tetramethinemerocyanine] iodide, magenta, 283.degree. (from C5H5N), IV; 5'-(3-methyl) p-toluenesulfonate analog, blue-green, 241.degree., V; 4'-(1-phenyl-3-methyl-5-pyrazolone) ptoluenesulfonate analog, green, 212.degree., VI; [2-(1-ethylquinoline)-5'-(3ethyl-2-thio-4- ketotetrahydrothiazole)-.gamma.2,''-(1ethylquinoline) tetramethinemerocyan ine] iodide, dark green, 204 degree., IV; 5'-(3-methyl) bromide analog, light green, 210.degree., V; 4'-(1-phenyl-3methyl-5-pyrazolone) analog, green, 260.degree., VI; 5'-(3-ethyl-2-thio-4ketotetrahydrooxazole) analog, light green, 248.degree., 3-ethyl-2-thio-4ketotetrahydrooxazole; [2-(3-ethylbenzoselenazole)-5'-(3-ethyl-2-thio-4ketotetrahydrothiazole) - .gamma.,2''-(3ethylbenzoselenazole)tetramethinemerocyanine] iodide, brown, 244.degree., IV; 5'-(3-methyl) analog, brassy green, 235.degree., V; 4'-(1-phenyl-3-methyl-5pyrazolone) analog, shiny green, 193.degree., VI. A dye intermediate 13 parts (prepd. from bis-2-(1,3,3- trimethylindolenine)pentamethinecyanine iodide) was

heated 5 min. with 2,3,3-trimethylindolenine-MeI (VII) 7.5 and Ac2O 400 parts, the cooled mixt. treated with Et20, and the pptd. tar solidified by trituration in Me2CO and crystd. from MeOH to give brown cryst. bis-2-(1,3,3trimethylindolenine) - .gamma.,2'-(1,3,3-trimethylindolenine)heptamethinecya nine diiodide, m. 238.degree.; 2-(3-ethylbenzothiazole) analog, dark brown, 214.degree., I; 2-(1-ethylquinoline) analog, dark blue, 213.degree., II; [5-(3-methyl-2-thio-4-ketotetrahydrothiazole)-2-(1,3,3- trimethylindolenine)-.beta.,2''-(1,3,3-trimethylindolenine)heptamethinemer ocyanine] iodide, royal blue, 209.degree., V (30 min. heating required); bis-2-(3-ethyl-5methylbenzothiazole) - .gamma., 2' - (3-ethyl-5methylbenzothiazole)heptamethinecyanine diiodide, dark blue, 213.degree., 1,6dimethylbenzothiazole-EtI; 2-(1-ethylquinoline)-2'-(3-ethyl-5methylbenzothiazole) - .gamma.,2''-(3-ethyl-5-methylbenzothiazole)heptamethi necyanine diiodide, green, 225.degree., II; 2-(1,3,3-trimethylindolenine) analog, dark green, 310.degree., VII; 2-(3-ethylbenzoxazole) analog, green, 222.degree., III; bis-2-(3-ethyl-5-chlorobenzothiazole)-.gamma.,2'- (3-ethyl-5-chlorobenzothiazole) heptamethinecyanine diiodide, green, 238.degree., 2methyl-5-chlorobenzothiazole-EtI; 2-(1-ethylquinoline)-2'- (3-ethyl-5chlorobenzothiazole) - .gamma., 2''-(3-ethyl-5- chlorobenzothiazole) heptamethinecyanine diiodide, dark green, 225.degree., II; and 2-(1,3,3trimethylindolenine) analog, light blue, 214.degree., VII. 878787-03-2P, Benzothiazolium, 2,2'-[5-[2-(1,3,3-trimethyl-2indolinylidene)ethylidene]-1,3-pentadienylene]bis[3-ethyl-5-methyliodide] 878787-04-3P, Benzothiazolium, 2,2'-[5-[2-(1,3,3trimethyl-2-indolinylidene)ethylidene]-1,3-pentadienylene]bis[5-chloro-3ethyl-, iodide RL: PREP (Preparation) (prepn. of) 878787-03-2 CAPLUS

Benzothiazolium, 2,2'-[5-[2-(1,3,3-trimethyl-2-indolinylidene)ethylidene]-

1,3-pentadienylene]bis[3-ethyl-5-methyl-iodide] (5CI) (CA INDEX NAME)

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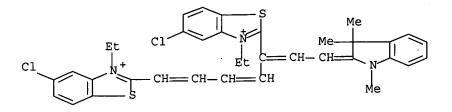
RN 878787-04-3 CAPLUS

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CN Benzothiazolium, 2,2'-[5-[2-(1,3,3-trimethyl-2-indolinylidene)ethylidene]-1,3-pentadienylene]bis[5-chloro-3-ethyl-, iodide (5CI) (CA INDEX NAME)



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